

**Amendments to the Claims:**

This listing of claims will replace all prior versions, and listings, of claims in the application:

**Listing of Claims**

Claim 1 (Currently Amended): A method for mining mass spectra, comprising:  
specifying spectral characteristics of ~~said a mass spectrum~~a mass spectrum to be mined;  
specifying a relationship between said spectral characteristics of said mass spectrum  
to be mined;

searching said mass ~~spectra~~spectrum for portions of said mass ~~spectra~~spectrum  
which match said spectral characteristics based on said relationship; and

assigning scores to said portions of said mass ~~spectra~~spectrum to indicate a degree of  
correlation between said portions of said mass ~~spectra~~spectrum and said spectral  
characteristics.

Claim 2 (Currently Amended): The method of claim 1, wherein said mass spectrum  
is spectra~~are~~ obtained by any one of dissociation and full-scan.

Claim 3 (Original): The method of claim 1, wherein the step of specifying spectral  
characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

Claim 4 (Original). The method of claim 1, wherein  
said step of specifying a relationship includes identifying each of said spectral  
characteristics as being one of a primary and a secondary spectral characteristic, said  
secondary spectral characteristic being linked hierarchically with said primary spectral  
characteristic and detected only after said primary spectral characteristic is detected.

Claim 5 (Currently Amended): The method of claim 3, wherein  
said step of specifying at least one of a product ion, a loss ion, and an ion series  
comprises specifying each of a product ion, a loss ion, and an ion series; and  
said assigning step includes:

- calculating a product ion score;
- calculating a loss ion score;
- calculating an ion series score;
- adjusting said product ion, loss ion, or said ion series score if respective said  
product ion, loss ion, or ion series spectral characteristic is secondary; and
- adding said product ion, loss ion, and ion series scores.

Claim 6 (Original): The method of claim 5, wherein the step of calculating a product  
ion score includes:

- identifying a most abundant ion within a window around said product ion spectral  
characteristic; and
- setting said product ion score as a percentage of total ion current of said identified ion.

Claim 7 (Original): The method of claim 5, wherein the step of calculating a loss ion  
score includes: calculating a loss ion mass per unit charge based on an actual precursor ion  
mass per unit charge and said loss ion spectral characteristic;

- identifying a most abundant ion within a window around said calculated loss ion mass  
per unit charge; and
- setting said loss ion score as a percentage of total ion current of said identified ion.

Claim 8 (Currently Amended): The method of claim 5, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;

generating hypothetical ions separated by said specified distances;

aligning said mass ~~spectra~~-spectrum with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned mass ~~spectra~~-spectrum at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 9 (Original): The method of claim 5, wherein said adjusting step includes:

setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

Claim 10 (Currently Amended): The method of claim 1, further comprising:

preprocessing said mass ~~spectra~~-spectrum; and displaying said scores from said assigning step.

Claim 11 (Currently Amended): The method of claim 10, wherein said preprocessing step includes:

subtracting nonfragment ions from said mass ~~spectra~~spectrum;  
estimating a precursor charge of mass ~~spectra~~spectrum resulting from said subtracting step; and  
normalizing an ion intensities-intensity of said mass ~~spectra~~spectrum from said estimating step as a percentage of a total ion current.

Claim 12 (Original): The method of claim 10, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

Claim 13 (Currently Amended): The method of claim 1, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said mass ~~spectra~~spectrum, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said mass ~~spectra~~spectrum.

Claim 14 (Currently Amended): The method of claim 1, further comprising:  
adjusting control parameters of a device that produces said mass ~~spectra~~spectrum  
based on said assigned scores.

Claim 15 (Currently Amended): A method for mining collision-induced dissociation (CID) spectra, comprising:

specifying spectral characteristics of said a CID ~~spectra~~spectrum to be mined;

specifying a relationship between said spectral characteristics of said CID spectrum  
to be mined;

searching said CID ~~spectra-spectrum~~ for portions of said CID ~~spectra-spectrum~~ which  
match said spectral characteristics based on said relationship; and

assigning scores to said portions of said CID ~~spectra-spectrum~~ to indicate a degree of  
correlation between said portions of said CID ~~spectra-spectrum~~ and said spectral  
characteristics.

Claim 16 (Original): The method of claim 15, wherein the step of specifying spectral  
characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

Claim 17 (Original). The method of claim 15, wherein  
said step of specifying a relationship includes identifying each of said spectral  
characteristics as being one of a primary and a secondary spectral characteristic, said  
secondary spectral characteristic being linked hierarchically with said primary spectral  
characteristic and detected only after said primary spectral characteristic is detected

Claim 18 (Previously Presented): The method of claim 16, wherein  
said step of specifying at least one of a product ion, a loss ion, and an ion series  
comprises specifying each of a product ion, a loss ion, and an ion series; and  
said assigning step includes:

calculating a product ion score;

calculating a loss ion score;

calculating an ion series score;

adjusting said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary; and  
adding said product ion, loss ion, and ion series scores.

Claim 19 (Original): The method of claim 18, wherein the step of calculating a product ion score includes:

identifying a most abundant ion within a window around said product ion spectral characteristic; and  
setting said product ion score as a percentage of total ion current of said identified ion.

Claim 20 (Original): The method of claim 18, wherein the step of calculating a loss ion score includes:

calculating a loss ion mass per unit charge based on an actual precursor ion mass per unit charge and said loss ion spectral characteristic;  
identifying a most abundant ion within a window around said calculated loss ion mass per unit charge; and  
setting said loss ion score as a percentage of total ion current of said identified ion.

Claim 21 (Currently Amended): The method of claim 18, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;  
generating hypothetical ions separated by said specified distances;  
aligning said CID ~~spectra~~spectrum with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned CID ~~spectra~~spectrum at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 22 (Original): The method of claim 18, wherein said adjusting step includes:  
setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

Claim 23 (Currently Amended): The method of claim 15, further comprising:  
preprocessing said CID ~~spectra~~spectrum; and displaying said scores from said assigning step.

Claim 24 (Currently Amended): The method of claim 23, wherein said preprocessing step includes:

subtracting nonfragment ions from said CID ~~spectra~~spectrum;

estimating a precursor charge of said CID ~~spectra~~spectrum resulting from said subtracting step; and

normalizing ion intensities of said CID ~~spectra~~spectrum from said estimating step as a percentage of a total ion current.

Claim 25 (Original): The method of claim 23, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

Claim 26 (Currently Amended): The method of claim 15, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said CID ~~spectra~~spectrum, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said CID ~~spectra~~spectrum.

Claim 27 (Currently Amended): The method of claim 15, further comprising:  
adjusting control parameters of a device that produces said CID spectrum based on said assigned scores.

Claim 28 (Currently Amended): A system for mining mass spectra, comprising:  
means for specifying spectral characteristics of ~~said a mass spectra~~spectrum to be mined;  
means for specifying a relationship between said spectral characteristics of said mass spectraum to be mined;  
means for searching said mass ~~spectra~~spectrum for portions of said mass ~~spectra~~spectrum which match said spectral characteristics based on said relationship; and  
means for assigning scores to said portions of said mass ~~spectra~~spectrum to indicate a degree of correlation between said portions of said mass ~~spectra~~spectrum and said spectral characteristics.



Claim 29 (Currently Amended): The system of claim 28, wherein said mass ~~spectra~~spectrum ~~are~~is obtained by any one of dissociation and full-scan.

Claim 30 (Currently Amended): The system of claim 28, further comprising:  
means for preprocessing said mass ~~spectra~~spectrum; and  
means for displaying said scores from said assigning means.

Claim 31 (Currently Amended): The system of claim 28, wherein the means for specifying spectral characteristics includes means for automatically specifying said spectral characteristics based on said mass ~~spectra~~spectrum, and  
wherein the means for specifying a relationship includes means for automatically specifying said relationship based on said mass ~~spectra~~spectrum.

Claim 32 (Currently Amended): The system of claim 28, further comprising:  
means for adjusting control parameters of a device that produces said mass ~~spectra~~spectrum based on said assigned scores.

Claim 33 (Currently Amended): A system, comprising:  
a memory device having embodied therein a mass ~~spectra~~-spectrum to be mined; and  
a processor in communication with the memory device, the processor configured to  
specify spectral characteristics of said mass ~~spectra~~spectrum to ~~identify~~be  
mined,  
specify a relationship between said spectral characteristics of said mass spectra  
to be mined,

search said mass spectraspectrum for portions of said mass spectraspectrum which match said spectral characteristics based on said relationship, and  
assign scores to said portions of said mass spectraspectrum to indicate a degree of correlation between said portions of said mass spectraspectrum and said spectral characteristics.

. Claim 34 (Currently Amended): A computer program product including a computer readable medium for mining mass spectraspectrum, comprising:

a graphical user interface code configured to allow a user to input spectral characteristics of a mass spectrum to be mined and to specify a relationship between said spectral characteristics; and

a mining code configured to search said mass spectraspectrum for portions of said mass spectraspectrum matching said spectral characteristics based on said relationship and assign scores to said portions of said mass spectraspectrum to indicate a degree of correlation between said portions of said mass spectraspectrum and said spectral characteristics.

Claim 35 (Currently Amended): The computer program product of claim 34, wherein said mass spectraspectrum are obtained by any one of dissociation and full-scan.

Claim 36 (Original). The computer program product of claim 34, wherein the graphical user interface code is configured

to accept at least one of a product ion, a loss ion, and an ion series as an input, identify said spectral characteristics as being one of a primary and a secondary spectral characteristic, and

link said secondary spectral characteristic with said primary spectral characteristic such that said secondary spectral characteristic is detected only after said primary spectral characteristic is detected

Claim 37 (Currently Amended): The computer program product of claim 34, wherein the graphical user interface code comprises:

a control window configured to input the spectral characteristics and the relationship between said spectral characteristics of said mass ~~spectra~~spectrum; and  
a results window configured to display said scores of said mass ~~spectra~~spectrum.

Claim 38 (Previously Presented): The computer program product of claim 34, wherein

said at least one of a product ion, a loss ion, and an ion series comprises each of a product ion, a loss ion, and an ion series; and

the mining code is configured to

calculate a product ion score,

calculate a loss ion score,

calculate an ion series score,

adjust said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary, wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked, and  
add said product ion, loss ion, and ion series scores.

Claim 39 (Currently Amended): The computer program product of claim 38,  
wherein said mining code is further configured to

calculate the product ion score by identifying a most abundant ion within a window  
around said product ion spectral characteristic and setting said product ion score as a  
percentage of total ion current of said identified ion,

calculate the loss ion score by calculating a loss ion mass per unit charge based on an  
actual precursor ion mass per unit charge and said loss ion spectral characteristic, identifying  
a most abundant ion within a window around said calculated loss ion mass per unit charge,  
and setting said loss ion score as a percentage of total ion current of said identified ion, and

calculate the ion series score by specifying distances between ions in an ion series as  
the ion series spectral characteristic, generating hypothetical ions separated by said specified  
distances, aligning said mass ~~spectra~~spectrum with said hypothetical ions, identifying most  
abundant ions within respective windows around said aligned mass ~~spectra~~spectrum at said  
specified distances, and setting said ion series score as a geometric mean of a percentage of  
total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \cdot \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions  
and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 40 (Currently Amended): The computer program product of claim 34, further  
comprising:

a preprocessing code configured to process said mass ~~spectra~~spectrum prior to mining  
in order to remove spurious mass spectra data.

Claim 41 (Currently Amended): The computer program product of claim 40, wherein the preprocessing code is configured to

subtract nonfragment ions from said mass ~~spectra~~spectrum,

estimate a precursor charge of said mass ~~spectra~~spectrum resulting from said subtracting step, and

normalize an ion ~~intensities~~-intensity of said mass ~~spectra~~spectrum from said estimating step as a percentage of a total ion current.

Claim 42 (Original): The computer program product of claim 37, wherein the graphical user interface code further comprises:

a product ion window configured to input said product ion spectral characteristic;

a loss ion window configured to input said loss ion spectral characteristic; and

an ion series window configured to input said ion series spectral characteristic,

wherein said product ion, loss ion, and ion series windows open when respective said spectral characteristics are selected in said control window.

Claim 43 (Original): The computer program product of claim 37, wherein said results window displays said scores in one of tabular and graphical form.

Claim 44 (Currently Amended): The computer program product of claim 34, wherein the graphical user interface code is configured to accept automatically specified said spectral characteristics and said relationship based on said mass ~~spectra~~spectrum.

Claim 45 (Currently Amended): The computer program product of claim 34, further comprising:

a control code configured to adjust control parameters of a device which generates said mass ~~spectra~~spectrum based on said assigned scores.

Claim 46 (Original): A computer readable medium containing program instructions for execution on a computer system, which when executed by the computer system, cause the computer system to perform the method recited in any one of claims 1 through 14.

Claim 47 (Currently Amended): A graphical user interface, comprising:

a control window configured to input spectral characteristics of a mass spectrum to be mined and a relationship between said spectral characteristics ~~of mass spectra~~; and

a results window configured to display scores of said mass ~~spectra~~spectrum indicating how well said mass ~~spectra~~spectrum match said spectral characteristics.

Claim 48 (Original): The graphical user interface of claim 47, wherein said results window displays said scores in one of tabular and graphical form.